Lift-Off Fellowship report: Adsorption of self-avoiding walks

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A self-avoiding walk (SAW) ω on a graph G is a sequence of vertices $(\omega_0, \omega_1, \omega_2, \ldots)$ such that ω_i and ω_{i+1} are adjacent on G and $\omega_i \neq \omega_j$ for $i \neq j$. Though any graph G will suffice, SAWs are most frequently considered to live on infinite lattices like $\mathbb{Z}^d$ or the honeycomb lattice $\mathbb{H}$. SAWs were originally conceived [6] as a model of long-chain polymers in solution. Their advantage over the simpler random walk model is that they encapsulate the *excluded volume principle* — the fact that two unit pieces (monomers) of a polymer cannot occupy the same point in space.

While the study of SAWs has long since spread from theoretical chemistry and statistical mechanics to combinatorics and computer science, its usefulness as a modeling tool remains as great as ever. One physical phenomenon which is well suited to such an approach is polymer *adsorption* — the process by which polymers in solution interact with interfaces in their environment. Such interfaces can be impenetrable (for example, the glass wall of a test-tube) or penetrable (like the interface between two liquids of different densities). As temperature varies, polymers are sometimes observed to undergo a *phase transition*, where they stick (*adsorb*) to a surface at low temperatures but are repelled (*desorb*) from the same surface at high temperatures. The temperature at which this changeover occurs is called the *critical temperature*.

I used my AustMS Lift-Off Fellowship to continue research into SAW models of polymer adsorption which I began in my PhD thesis. This research was undertaken at the Department of Mathematics and Statistics at the University of Melbourne, where I also completed my PhD.

There were two main problems I was investigating. The first involves SAWs on the honeycomb lattice. This lattice is set apart from all other regular lattices in two or more dimensions, in that there are a number of exact results regarding SAWs which have been conjectured or proved — most notably, the exact value of the connective constant [5]. There are two natural ways to orient an impenetrable surface on this lattice, and for each of these orientations there exists a conjecture for the critical surface fugacity (related to temperature by an energy term) of adsorbing SAWs [1], [2]. One of these two results was proven during my PhD [4]; I proved the second in the time between submitting my thesis and taking up a post-doctoral position in France [3]. This result was largely an adaptation of our first paper, which in turn generalised some key results obtained by Duminil-Copin and Smirnov. There were however a number of subtle complications which needed to be overcome.

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The second problem I was looking at involved some solvable models of SAW adsorption. Here, we look at subclasses of SAWs which have certain additional properties, which enable us to exactly solve their generating functions. In the past, the kinds of subclasses considered usually obeyed some kind of *directedness* restriction, where walks are forbidden from stepping in a certain direction on the lattice (for example, walks on $\mathbb{Z}^2$ might be forbidden from stepping in the negative x direction). I was looking at several models on the square (i.e. $\mathbb{Z}^2$) and triangular lattices which do not have a directedness restriction, and are thus able to take steps in all directions on their respective lattices (four for the square lattice and six for the triangular). They are instead *prudent walks*, which are forbidden from taking a step towards a vertex already visited by the walk. I have solved the generating functions for a number of these models, and after detailed analysis have discovered some unusual behaviour at the critical point. In particular, the order of the phase transition (essentially a measurement of how smoothly adsorption occurs) depends on the location of the endpoints of a walk; this is not the case for the previously solved directed models. This research is still ongoing.

The support provided to me by AustMS has been immensely helpful in allowing me to continue researching after my PhD, and so I thank them as well as strongly encouraging other PhD students nearing the end of their candidature to take advantage of this great opportunity.

References

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Nicholas completed a Bachelor of Science (Honours) at the University of Queensland in 2008 with an Honours thesis on block designs. He completed his PhD at the University of Melbourne in 2012 under the supervision of Professor Tony Guttmann, with a thesis titled *Combinatorics of Lattice Paths and Polygons*. He is currently working as a postdoctoral researcher at the Laboratoire d'Informatique du Paris-Nord at Université Paris 13, France.